

A FICK-JACOBS EQUATION FOR CHANNELS OVER 3D CURVES

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ABSTRACT. The purpose of this paper is to provide a new formula for the effective diffusion coefficient of a generalized Fick-Jacobs equation for narrow 3-dimensional channels. The generalized Fick-Jacobs equation is obtained by projecting the 3-dimensional diffusion equation along the normal directions of a curve in three dimensional space that roughly resembles the narrow channel. The projection (or dimensional reduction) is achieved by integrating the diffusion equation along the cross sections of the channel contained in the planes orthogonal to the curve. We show that the resulting formula for the associated effective diffusion coefficient can be expressed in terms of the geometric moments of the channel's cross sections and the curve's curvature. We show the effect that a rotating cross section with offset has on the effective diffusion coefficient.

1. INTRODUCTION

Understanding spatially constrained diffusion in quasi-one dimensional systems is of fundamental importance in various sciences, such as biology (e.g. channels in biological systems), chemistry (e.g. pores in zeolites) and nano-technology (e.g. carbon nano-tubes). However, solving the diffusion equation in arbitrary channels is a very difficult task. One way to tackle it, which we follow in this paper, consists in reducing the degrees of freedom of the problem by considering only the main direction of transport.

The study of diffusion in (nearly) planar narrow channels has been undertaken and developed by several authors [1, 2, 3] following the approach of reducing the dimensionality of the problem to one dimension. They have provided formulas for estimates of the effective diffusion coefficient by "projecting" the two dimensional diffusion equation onto a straight line. More recently (see [4]), we have generalized this work by projecting the 2-dimensional diffusion onto an arbitrary curve on the plane, thus providing estimates of the effective diffusion coefficient involving the geometrical information of the curve (i.e. its curvature).

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In all the work mentioned above we can distinguish two cases: the infinite transversal diffusion rate case and the finite transversal diffusion rate case. In the former, it is assumed that the concentration distribution stabilizes instantly in the transversal directions of the channel and, in the latter, the finite time of transversal stabilization is taken into account. In mathematical terms this cases can be characterized as follows. In the first case the effective diffusion coefficient only involves 0-th order geometrical quantities of the channel (such as width). In the second case this coefficient involves higher order geometrical information, such as that arising from the tangential and curvature information (i.e. higher derivatives) of the channel's surface wall(s).

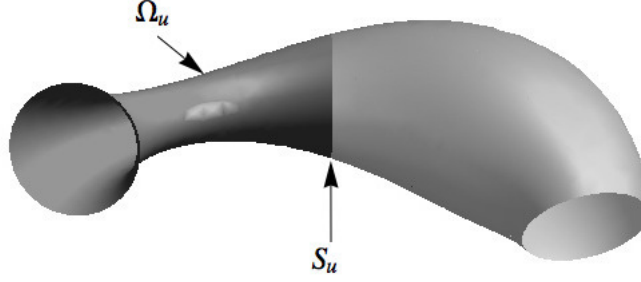
On the other hand, the diffusion process in 3-dimensional (non-planar) channels presents more complications and remains a difficult problem to tackle. Some attempts have been carried out by Ogawa [5], Kalinay & Percus [1], Antipov et al [6]. Ogawa derived a formula for the effective diffusion coefficient for channels in 3-dimensional space over a central curve with constant rectangular cross section, and showed that the curvature of the central curve plays a fundamental role. Kalinay and Percus studied the case of a hyperboloidal cone. Antipov et al. studied the case of a periodically expanding and contracting straight channel.

The main motivation for using arbitrary curves in the dimensionality reduction technique is the following: by choosing a curve that "follows" the channel's geometry as closely as possible, one is able to provide better estimates of the effective diffusion coefficient. In fact, we have shown in [4] that for two dimensional channels which are symmetric and of constant width, the formulas for the effective diffusion coefficient coincide in the finite and infinite transversal diffusion rate cases. In [5] Ogawa proved the same result for 3-dimensional channels having constant rectangular cross section.

Thus, the purpose of this paper is to derive a new formula for the effective diffusion coefficient (in the infinite transversal diffusion rate case) for 3-dimensional channels defined around a central curve in 3-dimensional space whose orthogonal cross section is not necessarily constant. We derive a formula for the effective diffusion coefficient with dependence on the curvature of the base curve, and the geometric and "statistical" properties of the cross section (i.e. its geometric moments). In particular, we derive explicit formulas relating the effective diffusion coefficient to the average widths and average rotation of the cross section of the channel with respect to the Frenet-Serret moving frame of the curve.

The outline of our article is as follows:

- In section 2, we will show how the three dimensional continuity equation on a channel can be reduced to a one dimensional continuity equation. This last equation, which we will call the effective continuity equation, will serve as the basis for what follows in the rest of the article.
- In section 3, we will derive a generalized Fick-Jacobs equation and a new formula for the effective diffusion coefficient \mathcal{D} corresponding to the infinite transversal diffusion rate case (see formula (3.9)). The standard Fick-Jacobs equation corresponds to the case when the base curve has zero curvature (i.e. it is a straight line). We will use standard tools of differential geometry of 3-dimensional curves to write down the formula for \mathcal{D} .
- In section 4, we study channels with gyrating cross section and deduce Ogawa's formula [5] as a particular case.

FIGURE 2.1. Region Ω_u and cross section S_u

- We finish with conclusions in section 5, a brief review of the necessary differential geometric material in Appendix 1, and in Appendix 2 we provide the details of the computations used to obtain some explicit formulas for the effective diffusion coefficient functions.

2. THE EFFECTIVE CONTINUITY EQUATION ON A 3-DIMENSIONAL REGION

We are interested in describing a transport process on a channel-like region Ω in 3-dimensional space (see Figure 2.1).

The continuity equation. Let us assume that this process is modelled by the continuity equation

$$(2.1) \quad \frac{\partial P}{\partial t} + \operatorname{div}(\mathbf{J}) = 0,$$

where $P = P(x, y, z, t)$ is a real valued density function and $\mathbf{J} = \mathbf{J}(x, y, z, t)$ is the corresponding flux field. We will apply a dimensionality reduction technique to this equation as follows. Let Ω be parametrized by a smooth map φ of the form

$$\varphi(u, v, w) = (x(u, v, w), y(u, v, w), z(u, v, w)),$$

where $u_1 \leq u \leq u_2, v_1 \leq v \leq v_2$ and $w_1 \leq w \leq w_2$. The parametrization φ allows us to express P and \mathbf{J} in terms of the u, v, w coordinates by letting

$$\begin{aligned} P(u, v, w, t) &= P(x(u, v, w), y(u, v, w), z(u, v, w), t), \\ \mathbf{J}(u, v, w, t) &= \mathbf{J}(x(u, v, w), y(u, v, w), z(u, v, w), t). \end{aligned}$$

For each u we will let Ω_u be the sub-region of Ω consisting of the points of the form $\varphi(s, v, w)$ such that $u_1 \leq s \leq u$, and S_u be the cross section parametrized by the map $(v, w) \mapsto \varphi(u, v, w)$ (see Figure 2.1).

Dimensional reduction of the continuity equation. From calculus in several variables, the total concentration of P in Ω_u is given by

$$C(u, t) = \int_{u_1}^u \left(\int_{w_1}^{w_2} \int_{v_1}^{v_2} P(s, v, w, t) \det(\varphi'(s, v, w)) dv dw \right) ds,$$

where φ' is the Jacobian matrix of φ . The *effective density* p is defined as

$$(2.2) \quad p(u, t) = \frac{dC}{du}(u, t) = \int_{w_1}^{w_2} \int_{v_1}^{v_2} P(u, v, w, t) \det(\varphi'(u, v, w)) dv dw$$

and the *effective flux* j by

$$j(u, t) = \int_{w_1}^{w_2} \int_{v_1}^{v_2} \mathbf{J}(u, v, w, t) \cdot \left(\frac{\partial \varphi}{\partial v}(u, v, w) \times \frac{\partial \varphi}{\partial w}(u, v, w) \right) dv dw,$$

where we have denoted the dot product by \cdot and the cross product by \times . The quantity $p(u, t)$ measures the concentration density at time t along the cross section S_u , and $j(u, t)$ measures the flux density along S_u . Let $\partial\Omega$ denote the border of the region Ω and assume that there is no flux of P across $\partial\Omega - (S_{u_1} \cup S_{u_2})$. Then by using the continuity equation (2.1) and the divergence theorem we obtain the effective continuity equation

$$(2.3) \quad \frac{\partial p}{\partial t}(u, t) + \frac{\partial j}{\partial u}(u, t) = 0.$$

Diffusion equation. By imposing Fick's law

$$\mathbf{J} = -D \nabla P,$$

where ∇P denotes the gradient of P in the spatial directions and D is a constant diffusion coefficient, the continuity equation (2.1) becomes *the diffusion equation*

$$\frac{\partial P}{\partial t} = D \Delta P,$$

where Δ is the laplacian operator given by

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

In this case, the 1-dimensional effective flux becomes

$$(2.4) \quad j(u, t) = -D \int_{w_1}^{w_2} \int_{v_1}^{v_2} \nabla P(u, v, w, t) \cdot \left(\frac{\partial \varphi}{\partial v}(u, v, w) \times \frac{\partial \varphi}{\partial w}(u, v, w) \right) dv dw,$$

where

$$\nabla P(u, v, w, t) = \left(\frac{\partial P}{\partial x}(\varphi(u, v, w), t), \frac{\partial P}{\partial y}(\varphi(u, v, w), t), \frac{\partial P}{\partial z}(\varphi(u, v, w), t) \right).$$

3. A GENERALIZED FICK-JACOBS EQUATION ON THE NORMAL BUNDLE OF A 3-DIMENSIONAL CURVE : INFINITE TRANSVERSAL DIFFUSION RATE CASE

In this section we derive a generalized Fick-Jacobs equation and a new formula for the effective diffusion coefficient (corresponding to the infinite transversal diffusion rate) for channels that "follow" a base curve in 3-dimensional space.

Channel set-up. Let $\alpha = \alpha(u)$ be a curve in three dimensional space parametrized by the arc-length parameter u , and consider scalar functions $\eta = \eta(u, v, w), \beta = \beta(u, v, w)$. Let Ω be the channel-like region parametrized by the map

$$(3.1) \quad \varphi(u, v, w) = \alpha(u) + \eta(u, v, w)\hat{N}(u) + \beta(u, v, w)\hat{B}(u),$$

where \hat{N} and \hat{B} are the normal and binormal fields of α (see Appendix 1). In this case, each cross section S_u is contained in the plane passing through $\alpha(u)$ and spanned by the vectors $\hat{N}(u)$ and $\hat{B}(u)$. By having arbitrary smooth functions β and η as coefficients we can generate very general cross sections S_u . By using the Frenet-Serret formulae we obtain

$$\begin{aligned} \frac{d\varphi}{du} &= (1 - \eta\kappa)\hat{T} + \left(\frac{\partial\eta}{\partial u} - \beta\tau\right)\hat{N} + \left(\frac{\partial\beta}{\partial u} + \eta\tau\right)\hat{B}, \\ \frac{\partial\varphi}{\partial v} &= \frac{\partial\eta}{\partial v}\hat{N} + \frac{\partial\beta}{\partial v}\hat{B}, \\ \frac{\partial\varphi}{\partial w} &= \frac{\partial\eta}{\partial w}\hat{N} + \frac{\partial\beta}{\partial w}\hat{B}, \end{aligned}$$

where κ and τ are the curvature and torsion functions associated to α . Since \hat{T}, \hat{N} and \hat{B} form an orthonormal basis, the derivative φ' of φ can be represented by the following matrix

$$[\varphi'] = \begin{pmatrix} 1 - \eta\kappa & \frac{\partial\eta}{\partial u} - \beta\tau & \frac{\partial\beta}{\partial u} + \eta\tau \\ 0 & \frac{\partial\eta}{\partial v} & \frac{\partial\beta}{\partial v} \\ 0 & \frac{\partial\eta}{\partial w} & \frac{\partial\beta}{\partial w} \end{pmatrix},$$

so that

$$(3.2) \quad \det(\varphi') = \omega_S(1 - \eta\kappa),$$

where

$$\omega_S = \det \begin{pmatrix} \frac{\partial\eta}{\partial v} & \frac{\partial\eta}{\partial w} \\ \frac{\partial\beta}{\partial v} & \frac{\partial\beta}{\partial w} \end{pmatrix},$$

and

$$(3.3) \quad \frac{\partial\varphi}{\partial v} \times \frac{\partial\varphi}{\partial w} = \omega_S \hat{T}.$$

The map $(v, w) \mapsto \omega_S(u, v, w)$ is the area density function of the cross section S_u , so that

$$A(u) = \int_{w_1}^{w_2} \int_{v_1}^{v_2} \omega_S(u, v, w) dv dw.$$

is the area of S_u . Given a function $f = f(v, w)$, its integral on S_u is given by

$$\int_{S_u} f = \int_{w_1}^{w_2} \int_{v_1}^{v_2} f(v, w) \omega_S(u, v, w) dv dw,$$

i.e. we integrate f over S_u by using the area element $\omega_S(u, v, w) dv dw$. The average value of f over S_u is then expressed as

$$\langle f \rangle_u = \frac{1}{A(u)} \int_{S_u} f.$$

In order to simplify notation, we will write $\langle f \rangle$ for the function $u \mapsto \langle f \rangle_u$.

Infinite transversal diffusion rate. The assumption of *infinite transversal diffusion rate* means that P is independent of the variables v and w . In this case, we have that the effective density (2.2) is given by

$$(3.4) \quad p(u, t) = \omega(u)P(u, t)$$

where

$$\omega(u) = \int_{v_1}^{v_2} \int_{w_1}^{w_2} \det(\varphi'(u)) dv dw.$$

The function $\omega(u)$ is the volume density function with respect to u , so that

$$V(u) = \int_{u_0}^u \omega(s) ds$$

is the volume of the region Ω_u . By using formula (3.2) we obtain

$$\begin{aligned} \omega(u) &= \int_{S_u} (1 - \kappa\eta) \\ &= A(u)(1 - \kappa(u)\langle\eta\rangle_u). \end{aligned}$$

To compute the effective flux (2.4) observe that P is constant along the planes passing through $\alpha(u)$ and spanned by $\hat{N}(u)$ and $\hat{B}(u)$. Hence ∇P is orthogonal to \hat{N} and \hat{B} so that

$$\begin{aligned} \frac{\partial P}{\partial u} &= \nabla P \cdot \frac{\partial \varphi}{\partial u} \\ &= (1 - \eta\kappa) \nabla P \cdot \hat{T}, \end{aligned}$$

where ∇P is the gradient of P with respect to the x, y, z variables. Using this and formulas (2.4) and (3.3), we obtain

$$(3.5) \quad j(u, t) = -D \frac{\partial P}{\partial u}(u, t) \int_{S_u} (1 - \eta\kappa)^{-1},$$

where κ only depends on u . By using equation (3.4) and letting

$$\begin{aligned} (3.6) \quad \mathcal{D}(u) &= D \left(\frac{\int_{S_u} (1 - \kappa\eta)^{-1}}{\int_{S_u} (1 - \kappa\eta)} \right) \\ &= D \left(\frac{\langle (1 - \kappa\eta)^{-1} \rangle_u}{1 - \kappa\langle\eta\rangle_u} \right), \end{aligned}$$

formula (3.5) for j can be written as

$$(3.7) \quad j(u, t) = -\mathcal{D}(u)\omega(u) \frac{\partial}{\partial u} \left(\frac{p(u)}{\omega(u)} \right).$$

Generalized Fick-Jacobs equation and effective diffusion coefficient. If we substitute formula (3.7) into the effective continuity equation (2.3) we obtain the following *generalized Fick-Jacobs equation*

$$(3.8) \quad \frac{\partial p}{\partial t}(u, t) = \frac{\partial}{\partial u} \left(\mathcal{D}(u)\omega(u) \frac{\partial}{\partial u} \left(\frac{p(u, t)}{\omega(u)} \right) \right),$$

which, in turn, casts

$$(3.9) \quad \mathcal{D}(u) = D \left(\frac{\langle (1 - \kappa\eta)^{-1} \rangle_u}{1 - \kappa\langle\eta\rangle_u} \right).$$

as the *effective diffusion coefficient*.

Remark. When $\kappa = 0$, we have that $\mathcal{D} \equiv D$ and $\omega(u) = A(u)$, and the above generalized Fick-Jacobs becomes the classical Fick-Jacobs equation

$$\frac{\partial p}{\partial t}(u, t) = D \frac{\partial}{\partial u} \left(A(u) \frac{\partial}{\partial u} \left(\frac{p(u, t)}{A(u)} \right) \right).$$

Central curve. From the definition of φ we have that

$$\langle \varphi \rangle_u = \alpha(u) + \langle \eta \rangle_u \hat{N}(u) + \langle \beta \rangle_u \hat{B}(u).$$

Hence, $\langle \eta \rangle_u$ is the $\hat{N}(u)$ component of $\langle \varphi \rangle_u$ when taking $\alpha(u)$ as reference point. We will refer to the curve $\langle \varphi \rangle$ as the central curve of the channel defined by φ .

Remark. Since the volume of the region Ω_u is given by

$$V(u) = \int_{u_1}^u A(u) (1 - \kappa(u) \langle \eta \rangle_u) du,$$

when α and $\langle \varphi \rangle$ coincide, we have $\langle \eta \rangle \equiv 0$ and

$$V(u) = \int_{u_1}^u A(u) du.$$

For α a circle, the last formula is the well known Pappus theorem which establishes how to compute the volumes of solids of revolution.

Geometric moments. We can get a better understanding of the function $\langle (1 - \eta\kappa)^{-1} \rangle$ appearing in the numerator of \mathcal{D} , by considering the geometric series expansion

$$(1 - \eta\kappa)^{-1} = \sum_{n=0}^{\infty} \eta^n \kappa^n.$$

Observe that the lower order terms in this series dominate when $\kappa\eta < 1$, i.e. when the η coordinates of the channel are far away from the focal points $\alpha + \hat{N}/\kappa$ of the base curve α . This last condition is consistent with our narrow channel assumption. Using the above expansion we can write

$$\langle (1 - \eta\kappa)^{-1} \rangle = \left(\sum_{i=0}^{\infty} \langle \eta^i \rangle \kappa^i \right),$$

We will refer to the functions $\langle \eta^i \rangle$ as the channel's η -moments. Hence, we can write

$$(3.10) \quad \mathcal{D}(u) = \left(\frac{D}{1 - \kappa(u) \langle \eta \rangle} \right) \sum_{i=0}^{\infty} \langle \eta^i \rangle \kappa^i.$$

Remark. Observe that when $\kappa = 0$, we have $\mathcal{D}(u) = D$, and hence all the geometric information provided by the η moments of the channel is lost. This is, in fact, a good reason why to study the projection of diffusion along general (non-straight) curves.

The first three geometric moments. We will now use the first three terms in the series (3.10) to relate the effective diffusion coefficient \mathcal{D} to geometric properties of the channel. Consider the symmetric matrix

$$M(u) = \begin{pmatrix} a(u) & c(u) \\ c(u) & b(u) \end{pmatrix},$$

where

$$\begin{aligned} a &= \langle (\eta - \langle \eta \rangle)^2 \rangle, \\ b &= \langle (\beta - \langle \beta \rangle)^2 \rangle, \\ c &= \langle (\eta - \langle \eta \rangle)(\beta - \langle \beta \rangle) \rangle. \end{aligned}$$

The eigenvectors and eigenvalues of $M(u)$ can be used to measure the average orientation angle $\theta(u)$ and average sizes $s_1(u)$ and $s_2(u)$ of the cross section S_u in the $\hat{\mathbf{N}}(u)$ and $\hat{\mathbf{B}}(u)$ directions with respect to its central point $\langle \varphi \rangle_u$ (see Figure 3.1). Let $\lambda_1(u)$ and $\lambda_2(u)$ be the ordered eigenvalues of $M(u)$ such that $\lambda_1(u) \geq \lambda_2(u)$. The angle $\theta(u)$ is the one formed between $\hat{\mathbf{N}}(u)$ and the eigenvector of $M(u)$ corresponding to $\lambda_1(u)$, and the functions s_1 and s_2 are given by the formulas

$$s_1(u) = 2\sqrt{\lambda_1(u)} \quad \text{and} \quad s_2(u) = 2\sqrt{\lambda_2(u)}.$$

Some simple algebra then shows that

$$\begin{aligned} a &= \left(\frac{s_1}{2}\right)^2 \cos^2(\theta) + \left(\frac{s_2}{2}\right)^2 \sin^2(\theta), \\ b &= \left(\frac{s_2}{2}\right)^2 \cos^2(\theta) + \left(\frac{s_1}{2}\right)^2 \sin^2(\theta), \\ c &= \left(\left(\frac{s_1}{2}\right)^2 - \left(\frac{s_2}{2}\right)^2\right) \cos(\theta) \sin(\theta). \end{aligned}$$

Hence

$$\langle \eta^2 \rangle = \langle \eta \rangle^2 + \left(\frac{s_1}{2}\right)^2 \cos^2(\theta) + \left(\frac{s_2}{2}\right)^2 \sin^2(\theta).$$

Using the above formulas and the first three terms of the series (3.10) we obtain the following approximation

$$(3.11) \quad \mathcal{D} \approx \frac{D(1 + \langle \eta \rangle \kappa + \left(\langle \eta \rangle^2 + \left(\frac{s_1}{2}\right)^2 \cos^2(\theta) + \left(\frac{s_2}{2}\right)^2 \sin^2(\theta)\right) \kappa^2)}{(1 - \kappa \langle \eta \rangle)}.$$

Higher order moments. The higher order moments of η , i.e. the functions $\langle \eta^i \rangle$ for $i > 2$, contain more subtle information of the geometry of the channel than that provided by the moments of order 0, 1 and 2. For example, in the context of probability distributions concepts like skewness and kurtosis, which are a measure the asymmetry and "peakedness" of a distribution respectively, involve in their definition moments of order higher than two. These ideas can be carried onto the case of channels, where we would be talking about geometric distributions instead of probability distributions.

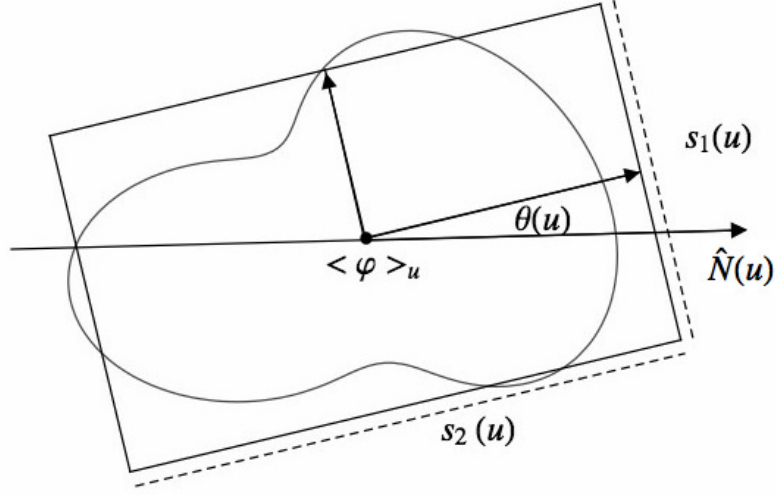


FIGURE 3.1. Average orientation and sizes of a channel's cross section with respect to $\langle \varphi \rangle$.

4. APPLICATIONS - TWISTED CHANNELS WITH OFFSETS

In this section we will apply our results to show how our formula for the effective diffusion coefficient captures information about the way the cross section of a channel gyrates with respect to the Frenet-Serret frame, as well as the effects of offsets from the base curve. We deduce Ogawa's formula [5] as a particular case.

We will consider a parametrisation φ of the form (3.1) where η and β are constructed as follows. For a fixed planar region R_0 parametrized by the map

$$(4.1) \quad (v, w) \mapsto (\eta_0(v, w), \beta_0(v, w)),$$

we let η, β be given by

$$(4.2) \quad \begin{pmatrix} \eta(u, v, w) \\ \beta(u, v, w) \end{pmatrix} = \begin{pmatrix} \cos(\omega u) & -\sin(\omega u) \\ \sin(\omega u) & \cos(\omega u) \end{pmatrix} \begin{pmatrix} \eta_0(v, w) \\ \beta_0(v, w) \end{pmatrix} + \begin{pmatrix} p(u) \\ q(u) \end{pmatrix}$$

For a given curve α , the parametrization φ with the above η and β , represents a channel constructed by rotating the region R_0 with angular velocity ω (as we move along the u -variable) with respect to the Frenet-Serret frame of α , and having offset $p(u)\hat{N}(u) + q(u)\hat{B}(u)$ from $\alpha(u)$.

4.1. Twisted elliptical cross sections with offsets. A solid ellipse with mayor and minor radii r_1 and r_2 can be parametrized by the map (4.1) with

$$\eta_0 = vr_1 \cos(w) \quad \text{and} \quad \beta_0 = vr_2 \sin(w),$$

for $0 \leq v \leq 1$ and $-\pi \leq w \leq \pi$. If we use η and β defined by formula (4.2), then the average sizes and the area of the channel's cross sections are given by

$$s_1 = r_1, s_2 = r_2 \quad \text{and} \quad A = \pi r_1 r_2.$$

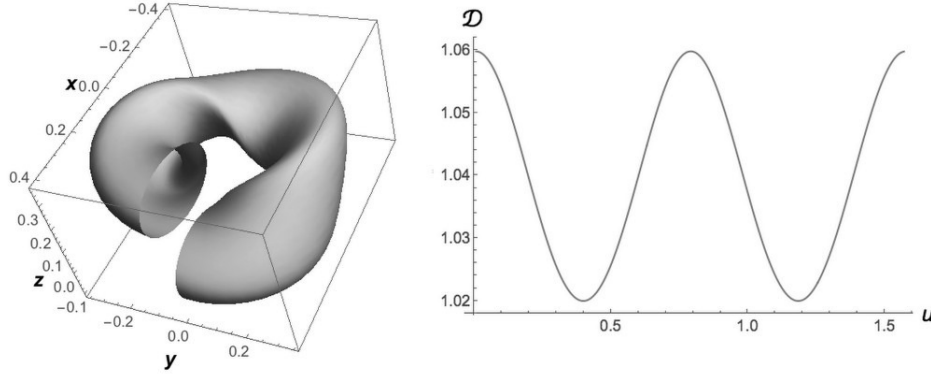


FIGURE 4.1. A twisted elliptical channel over a helix (left) and the corresponding effective diffusion coefficient function (right). The relevant parameters are: $D = 1, a = 1/4, b = 1/6, r_1 = 1/6, r_2 = 1/10, p = 0, q = 0$ and $\omega = 4$

In this case we can evaluate the integrals in formula (3.6) to obtain (see Appendix 2 for details)

$$(4.3) \quad \mathcal{D}(u) = \frac{2D}{(\kappa(u)R(u))^2} \left(1 - \frac{\sqrt{(1 - p(u)\kappa(u))^2 - (R(u)\kappa(u))^2}}{1 - \kappa(u)p(u)} \right),$$

where

$$R(u) = \sqrt{r_1^2 \cos^2(\omega u) + r_2^2 \sin^2(\omega u)}.$$

Observe that if there is no gyration and no offsets of the transversal cross sections, i.e. $\omega = p = q = 0$, then formula (4.3) for \mathcal{D} becomes

$$\mathcal{D}(u) = \frac{2D \left(1 - \sqrt{1 - r_1^2 \kappa^2(u)} \right)}{r_1^2 \kappa^2(u)}.$$

It is natural to ask how the terms in the series (3.10) approximate our formula (4.3). Due to the symmetry of the elliptical sections, the odd terms of this series vanish. Consider the curves shown in Figure 4.2 (counting them from the bottom to the top). The first curve shows the function obtained by truncating the series after the second term, which corresponds to formula (3.11). The second curve shows the function obtained by truncating the series after the fourth term. Finally, the top curve is the graph of the effective diffusion coefficient given by (4.3).

4.2. Twisted rectangular cross sections with offsets. A solid rectangle with sides d_1 and d_2 can be parametrized by a map of type (4.1) by letting

$$\eta_0 = v \quad \text{and} \quad \beta_0 = w,$$

where $-d_1/2 \leq v \leq d_1/2$ and $-d_2/2 \leq w \leq d_2/2$. We then have that

$$s_1 = d_1/\sqrt{3}, \quad s_2 = d_2/\sqrt{3} \quad \text{and} \quad A = d_1 d_2.$$

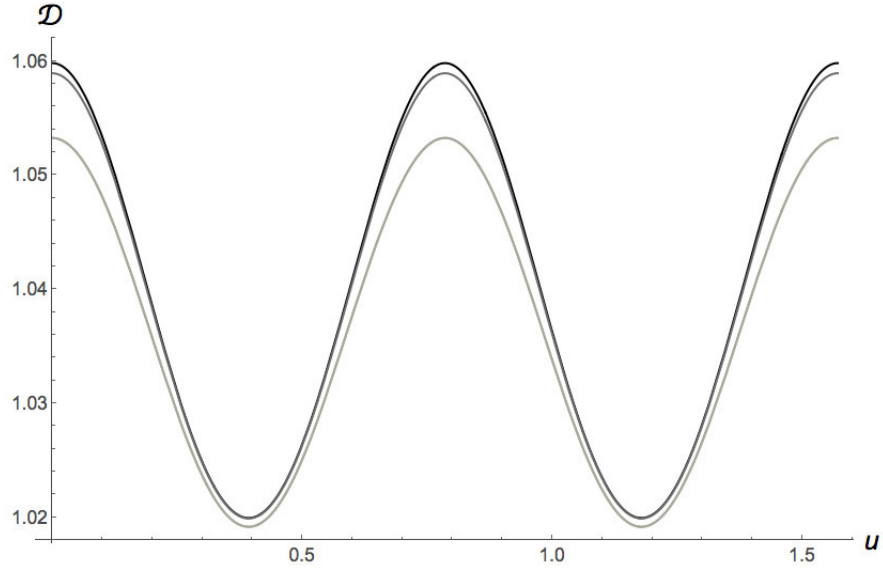


FIGURE 4.2. Geometric series approximation to the effective diffusion coefficient for a channel with gyrating elliptical cross section. The parameters used to generate these curves are the same as those in Figure 4.1

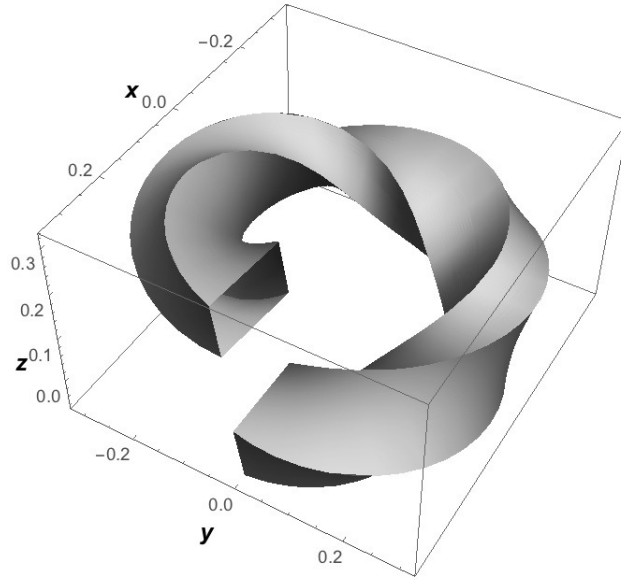


FIGURE 4.3. A twisted channel with rectangular cross section. The parameters used to generate the channel are $a = 1/4$, $b = 1/6$, $d_1 = 1/6$, $d_2 = 1/10$, $p = 0$, $q = 0$ and $\omega = 4$

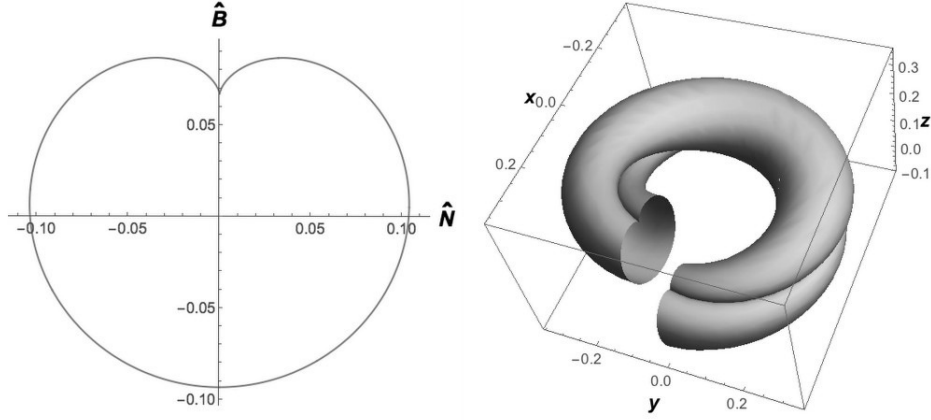


FIGURE 4.4. A twisted channel with cardioidal cross section. The parameters used to generate this channel are $a = 1/4, b = 1/6, r = 1/25, \omega = 4, p = 0, q = 0$.

In this case we can compute the integrals in formula (3.6) to obtain (see Appendix 2 for details)

$$(4.4) \quad \mathcal{D}(u) = \frac{D \left(\sum_{i=1}^4 (-1)^{i+1} \gamma_i(u) \log(\gamma_i(u)) \right)}{(d_1 d_2 \kappa(u))^2 (1 - \kappa(u) p(u)) \cos(\omega u) \sin(\omega u)},$$

where

$$\gamma_i(u) = 1 - \kappa(u)(p(u) - (\cos(\omega u), \sin(\omega u)) \cdot z_i)$$

and

$$z_1 = \frac{1}{2}(d_1, d_2), \quad z_2 = \frac{1}{2}(d_1, -d_2), \quad z_3 = \frac{1}{2}(-d_1, -d_2) \quad \text{and} \quad z_4 = \frac{1}{2}(-d_1, d_2).$$

When there is no gyration, i.e. $\omega = 0$, we have that

$$\mathcal{D}(u) = \frac{1}{\kappa(u) d_1} \log \left(\frac{1 + \kappa(u)(d_1/2 - p(u))}{1 - \kappa(u)(d_1/2 + p(u))} \right).$$

For $p = 0$, this formula is the one obtained by Ogawa in [5].

4.3. Twisted cardioidal cross sections with offsets. In this case we have that

$$\eta_0 = vr(2 \sin(w) - \sin(2w)) \quad \text{and} \quad \beta_0 = vr(2 \cos(w) - \cos(2w)) + (2/3)r,$$

where the parameter r is the radius of the circle used to construct the cardioidal curve. The interior of the region shown in the left part of Figure 4.4 is the region parametrized by the map $(v, w) \mapsto (\eta_0(v, w), \beta_0(v, w))$ for $0 \leq v \leq 1$ and $-\pi \leq w \leq \pi$. The right part of the figure shows the channel resulting from gyrating this cross section over the Frenet-Serret frame of a helix. Under the above hypotheses we obtain

$$s_1 = \sqrt{7}r, \quad s_2 = \frac{\sqrt{47}}{3}r \quad \text{and} \quad A = 6\pi r^2.$$

In this case, we use the series (3.10) to compute explicit formulas that approximate \mathcal{D} , and use numerical techniques to compute the integrals (3.6) in concrete examples.

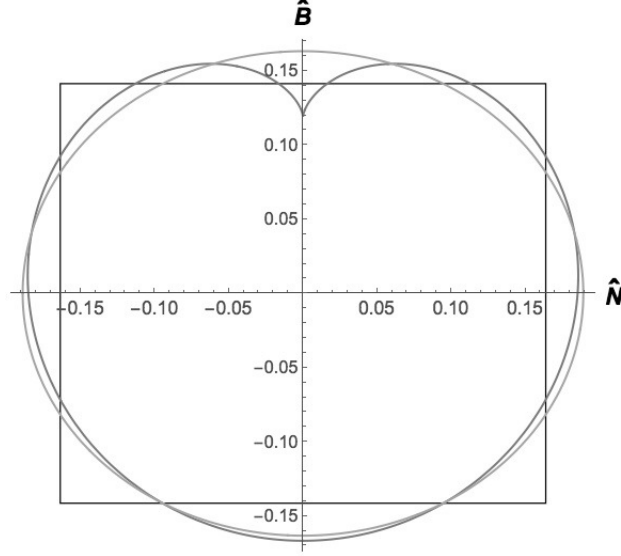


FIGURE 4.5. Elliptical, rectangular and cardioidal sections having the same width values s_1 and s_2 .

4.4. Comparing the elliptical, rectangular and cardioidal cases. We conclude by comparing the effective diffusion coefficients of the three types of twisted channels described above. To do a "fair" comparison we need to set the parameters of the cross sections so that their geometries are similar to second (geometric) order. We do this by equating their width functions s_1 and s_2 and their angle function θ . For a fixed value of the parameter r of the cardioid, the mayor and minor radii r_1 and r_2 of the elliptical cross section must be set to

$$(4.5) \quad r_1 = \sqrt{7}r \quad \text{and} \quad r_2 = \frac{\sqrt{47}}{3}r,$$

and the sides d_1 and d_2 of the rectangular cross section must be set to

$$(4.6) \quad d_1 = \sqrt{21}r \quad \text{and} \quad d_2 = \sqrt{\frac{47}{3}}r.$$

For the angle functions θ to be equal we simply need to use the same ω as the gyrating velocity in all cases.

We will illustrate the behaviour of the effective diffusion coefficients in these cases by letting

$$a = 1/4, b = 0, \omega = 4.$$

In Figure 4.6 we show the results obtained from the above selection of parameters by letting $r = 1/20$, and in Figure 4.7 the results obtained by letting $r = 1/15$. The effective diffusion formulas used in these examples are (4.3) and (4.4) for the elliptical and the rectangular case, and the cardioidal case was computed using numerical integration. To give an explanation of the behaviour just illustrated, we need the following description of the focal line.

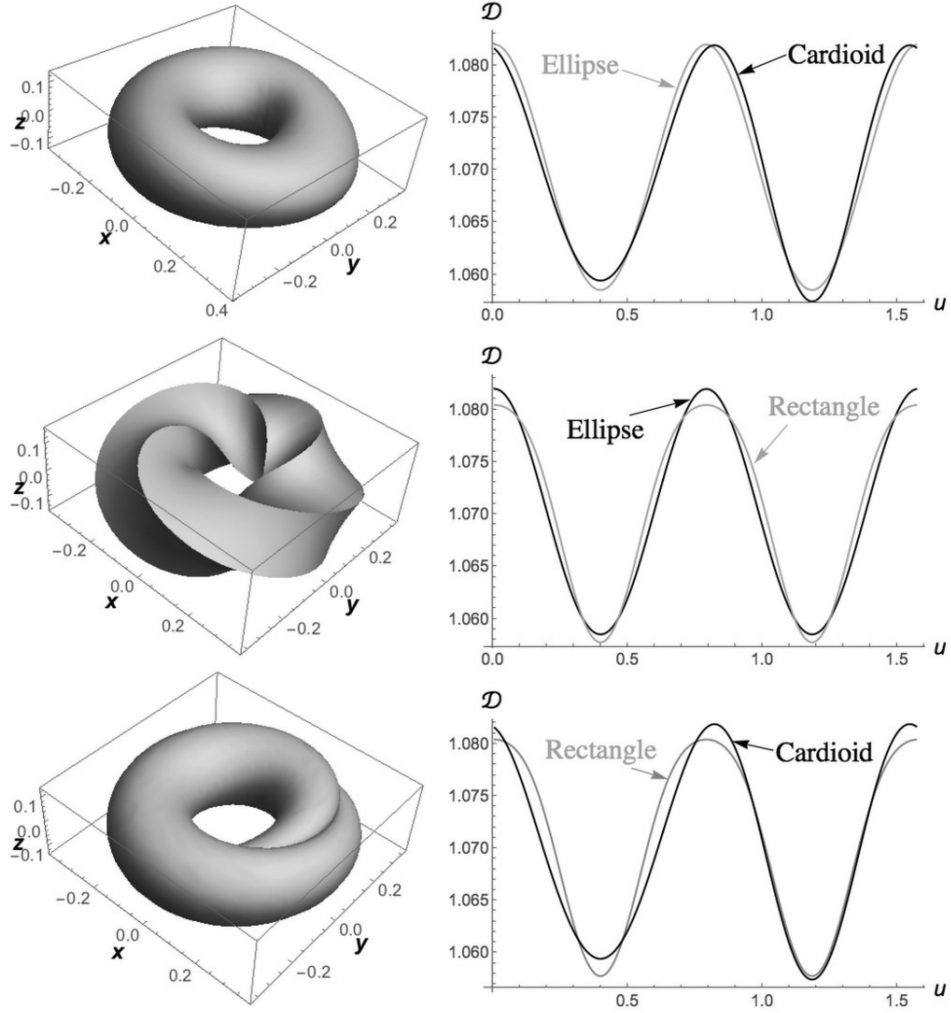


FIGURE 4.6. Pairwise comparisons of the effective diffusion coefficients for the twisted elliptical, rectangular and cardioidal channels with $r = 1/20$.

The focal line and the effective diffusion coefficient. The focal set of a 3-dimensional curve α consists of the points of the form $\alpha(u) + (1/\kappa(u))\hat{N}(u)$. The focal line through such a point is the one having direction $\hat{B}(u)$. The curve α used in the examples in Figures 4.6 and 4.7 is a circle in the xy -plane with radius a , and in this case the focal set consists of the origin $(0, 0, 0)$ and the corresponding focal lines have direction $\hat{B} = (0, 0, 1)$. For a given point $\mathbf{p} = \alpha(u) + \eta(u, v, w)\hat{N}(u) + \beta(u, v, w)\hat{B}(u)$ in a cross section S_u , the distance of \mathbf{p} to the corresponding focal line is

$$d_f(\mathbf{p}) = \frac{1 - \kappa(u)\eta(v, w)}{\kappa(u)}$$

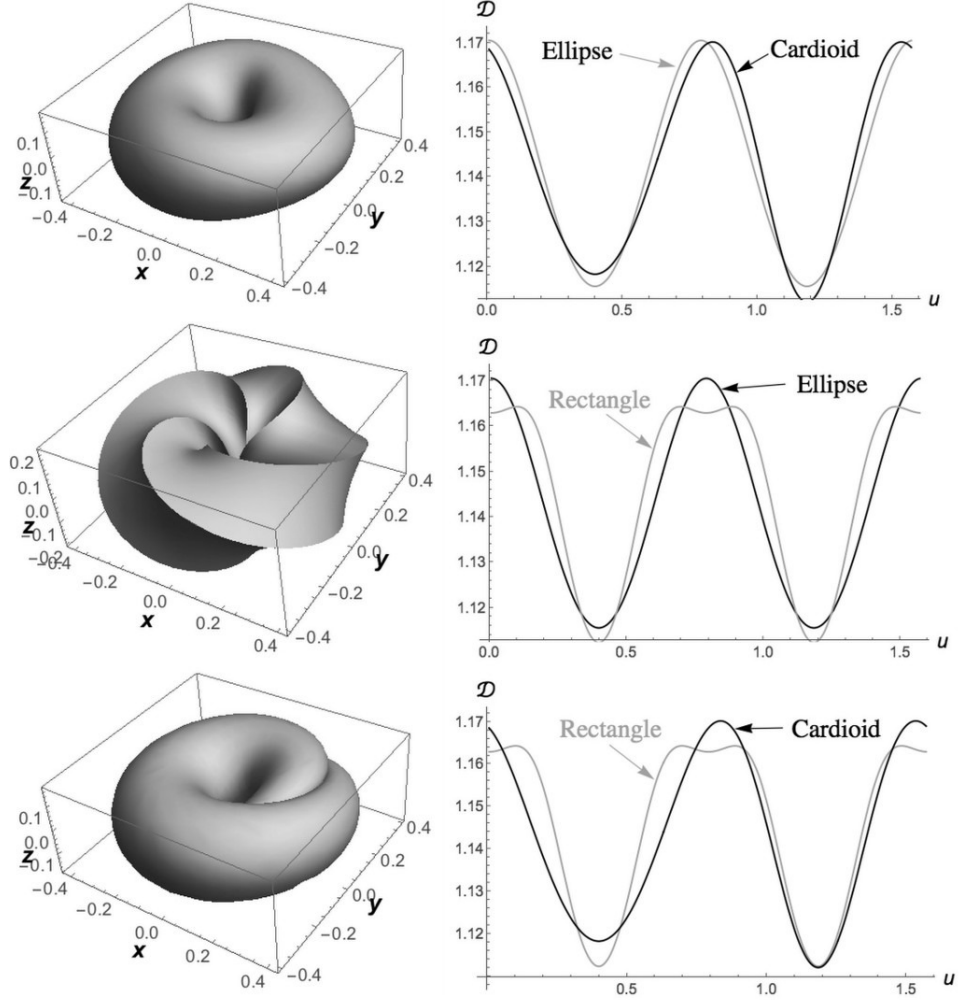


FIGURE 4.7. Pairwise comparisons of the effective diffusion coefficients for the twisted elliptical, rectangular and cardioidal channels with $r = 1/15$.

In order to simplify the arguments, let us assume that $\langle \eta \rangle = 0$ (which holds in our examples). Formula (3.6) can then be written as

$$(4.7) \quad \mathcal{D}(u) = \frac{1}{A(u)\kappa(u)} \int_{S_u} \frac{1}{d_f}.$$

Thus, we can make the following observations about the examples in Figures 4.6 and 4.7. The further away the cross section S_u is from the focal line, the less influence the geometry (geometric moments information) of the cross section has on $\mathcal{D}(u)$. Notice that in Figure 4.6 the effective diffusion coefficients look more similar to each other than in Figure 4.7, where the effective diffusion coefficient for the rectangular channel has developed extra "bumps" due to the proximity of

the channel to the focal line. As r tends to 0, the cross sections are further away from the focal line, and the effective diffusion coefficients look more similar to each other. In the limit when $r = 0$, all the effective diffusion coefficients become equal to $D = 1$.

Symmetries. We will now explain some of the features of the effective diffusion coefficients shown in Figures 4.6 and 4.7 in terms of the symmetries of the cross sections with respect to the normal field $\hat{\mathbf{N}}$. Observe that we have $0 \leq u \leq \pi/2$ and $\omega = 4$, so that the angle $\theta = \omega u$ covers a full cycle from 0 to 2π .

For $\theta = 0, \pi/2, \pi, 3\pi/2$ the ellipse is invariant under reflections with axis given by the normal vector $\hat{\mathbf{N}}$ at these points. This explains the four critical points of \mathcal{D} at $u = 0, \pi/8, \pi/4, 3\pi/8$. When $u = 0, \pi/4$ the mayor axis of the ellipse faces the focal line and the corresponding critical points are local maxima. When $u = \pi/8, 3\pi/8$ the minor axis of the ellipse faces the focal line and the corresponding critical points are local minima. This is consistent with our observation that the closer the cross section is to the focal line, the larger the effect it has on the effective diffusion coefficient.

For $\theta = \pi/2, 3\pi/2$ the cardioid is invariant under reflections with axis given by the normal vector $\hat{\mathbf{N}}$ at these points. This explains the two critical points of \mathcal{D} at $u = \pi/8, 3\pi/8$. These two points are local minima of \mathcal{D} , since the smallest axis of the cardioid faces the focal line for these angles. The first local minimum is smaller than the second because in the first case the "dent" of the cardioid is directed towards the focal line and in the second case this "dent" faces away from the focal line. The local maxima of \mathcal{D} appearing near $u = 0$ and $u = \pi/4$ can be explained again by the fact the largest axis of the cardioid faces the focal line at these angles, and the asymmetry of the the cardioid with respect to reflection along the normal line explains the fact that the u values at which this maxima occur, appear with offsets (to the left and right) to the exact values 0 and $\pi/4$.

The behaviour of the critical points in the rectangle case can be explained in a similar way as in the previous two cases, with the added effect (if the rectangle is close enough to the focal line) that the corners of the rectangle generate the "bumps" on the effective diffusion function (shown in Figure 4.7) as they get closer to the focal line.

5. CONCLUSIONS AND FUTURE WORK

We have deduced a new formula for the effective diffusion coefficient \mathcal{D} of a generalized Fick-Jacobs equation for narrow 3-dimensional channels. We derived such a formula by projecting the diffusion equation along the normal directions of a base curve of a narrow channel in 3-dimensional space under the assumption of infinite transversal diffusion rate, and using tools of differential geometry of curves. Our formula establishes an explicit relation between some of the channel's geometric properties (i.e. curvature of the base curve and the geometric moments of the transversal cross sections) and the corresponding effective diffusion coefficient. We have also showed that previous estimates [5] for \mathcal{D} can be recovered from our formula as particular cases, and how our formula captures information about the way the cross sections gyrate with respect to the Frenet-Serret frame.

In future work, we will deal with finite transversal diffusion rate case. We expect that in that case both tangential and curvature information of the channel's surface will enter into the formula of the effective diffusion coefficient.

6. APPENDIX 1 - THE FRENET-SERRET FORMULAS FOR 3D CURVES.

In this appendix we review some basic concepts of the differential geometry of curves in three dimensional space. The material is standard and can be found in books such as [7, 8]. Consider a smooth curve in three dimensional space of the form $\alpha(s) = (x(s), y(s), z(s))$. The curve is said to have arc-length parametrization if for all s in the interval $[s_1, s_2]$ we have that

$$\left| \frac{d\alpha}{ds} \right| = 1 \quad \text{where} \quad \left| \frac{d\alpha}{ds} \right| = \sqrt{\left(\frac{dx}{ds} \right)^2 + \left(\frac{dy}{ds} \right)^2 + \left(\frac{dz}{ds} \right)^2}.$$

If the above condition holds, then the length of the curve segment $\alpha([s_1, s])$ is given by

$$\text{length}(\alpha([s_1, s])) = \int_{s_1}^s \left| \frac{d\alpha}{ds}(a) \right| da = s.$$

We can construct three orthonormal fields to α given by

$$\hat{T} = \frac{d\alpha}{ds}, \hat{N} = \frac{d\hat{T}}{ds} / \left\| \frac{d\hat{T}}{ds} \right\| \quad \text{and} \quad \hat{B} = \hat{T} \times \hat{N},$$

which are known as the tangent, normal and bi-normal fields, respectively. The orthonormality conditions on these fields imply the existence of scalar functions $\kappa = \kappa(u)$ and $\tau = \tau(u)$, known as the curvature and torsion, such that

$$\begin{aligned} \frac{d\hat{T}}{ds} &= \kappa \hat{N}, \\ \frac{d\hat{N}}{ds} &= -\kappa \hat{T} + \tau \hat{B}, \\ \frac{d\hat{B}}{ds} &= -\tau \hat{N}. \end{aligned}$$

These formulas are known in the literature as the Frenet-Serret formulas, and the fields $\hat{T}, \hat{N}, \hat{B}$ as the Frenet-Serret frame. The curvature function measures the deviation of α of being a straight line, and τ the deviation of α from being in a plane.

As an example, consider a helix of radius $a > 0$ and pitch $b > 0$ parametrized by

$$s \mapsto (a \cos(s), a \sin(s), bs).$$

The arc-length parametrisation of this curve is

$$\alpha(u) = \left(a \cos \left(\sqrt{1 - b^2} u/a \right), a \sin \left(\sqrt{1 - b^2} u/a \right), bu \right),$$

and the corresponding curvature and torsion of this curve are

$$\kappa = \frac{a}{a^2 + b^2} \quad \text{and} \quad \tau = \frac{b}{a^2 + b^2}.$$

7. APPENDIX 2 - DETAILS ON THE COMPUTATION OF THE EFFECTIVE DIFFUSION COEFFICIENT

In our computation of the effective diffusion coefficient we have used the formula (3.6), which can be written (when $\langle \eta \rangle = p$) explicitly as

$$(7.1) \quad \mathcal{D}(u) = \left(\frac{D}{A(u)(1 - \kappa(u)p(u))} \right) \int_{v_1}^{v_2} \int_{w_1}^{w_2} \left(\frac{\omega_S(u, v, w)}{1 - \kappa(u)\eta(u, v, w)} \right) dv dw,$$

where

$$\omega_S(u, v, w) = \det \begin{pmatrix} \frac{\partial \eta}{\partial v}(u, v, w) & \frac{\partial \eta}{\partial w}(u, v, w) \\ \frac{\partial \beta}{\partial v}(u, v, w) & \frac{\partial \beta}{\partial w}(u, v, w) \end{pmatrix}.$$

For completeness, we will now expand some details regarding the computations of formulas (4.3) and (4.4) from (7.1). We calculate the above integral by using Fubini's Theorem. We do this by finding a function $H = H(u, v, w)$ such that

$$(7.2) \quad \frac{\partial H}{\partial v \partial w}(u, v, w) = \Omega(u, v, w),$$

where

$$(7.3) \quad \Omega(u, v, w) = \frac{\omega_S(u, v, w)}{1 - \kappa(u)\eta(u, v, w)}.$$

We then have

$$(7.4) \quad \mathcal{D}(u) = \left(\frac{D}{A(u)(1 - \kappa(u)p(u))} \right) \sum_{i,j=1}^2 (-1)^{i+j} H(v_i, w_j).$$

Elliptical case. The integrand function is

$$\Omega(u, v, w) = \frac{r_1 r_2 v}{1 - \kappa(u)(p(u) - r_2 v \sin(w) \sin(\omega u) + r_1 v \cos(w) \cos(\omega u))}.$$

From equation (7.2) we have that

$$\frac{\partial H}{\partial w} = \frac{r_1 r_2 (\kappa(p - \eta) - (1 - \kappa p) \log(2(1 - \kappa \eta)))}{\kappa^2 (p - \eta_1)^2},$$

where $\eta_1(u, w) = \eta(u, 1, w)$. We then obtain

$$(7.5) \quad H = \frac{r_1 r_2}{\kappa^2 R} \left((1 - \kappa p) \left(\frac{S \log(2(1 - \kappa \eta))}{p - \eta_1} + w \right) - 2Q \operatorname{arctanh}(T) \right)$$

where

$$\begin{aligned} R(u) &= r_1^2 \cos^2(\omega u) + r_2^2 \sin^2(\omega u) \\ Q(u, v) &= \sqrt{v^2 \kappa^2(u) R(u) - (1 - p(u) \kappa(u))^2} \\ T(u, v, w) &= \frac{(1 - \kappa(u)(p(u) - r_1 v \cos(\omega u)) \tan\left(\frac{w}{2}\right) + \kappa(u) r_2 v \sin(\omega u))}{Q(u, v)} \\ S(u, w) &= r_1 \sin(w) \cos(\omega u) + r_2 \cos(w) \sin(\omega u) \end{aligned}$$

By using formulas (7.4) and (7.5) we obtain (4.3).

When trying to directly evaluate the quantities $H(v_i, w_j)$ in formula (7.4) it turns out that they are not well defined for the values $w = -\pi, \pi$. We solve this problem by letting

$$H(v_i, \pi) = \lim_{w \rightarrow \pi^-} H(v_i, w) \quad \text{and} \quad H(v_i, -\pi) = \lim_{w \rightarrow -\pi^+} H(v_i, w)$$

Rectangular case. The integrand function is

$$\Omega(u, v, w) = \frac{d_1 d_2}{4 \left(1 - \kappa(u) \left(p(u) + \frac{1}{2} d_1 v \cos(\omega u) - \frac{1}{2} d_2 w \sin(\omega u) \right) \right)}.$$

From equation (7.2) we have that

$$\frac{\partial H}{\partial w} = - \frac{d_2 \log(2(1 - \kappa\eta))}{2\kappa \cos(\omega u)}$$

and

$$(7.6) \quad H = \frac{\log(2(1 - \eta\kappa))(d_1 \kappa v \cot(\omega u) - d_2 \kappa w + 2(\gamma\kappa - 1) \csc(\omega u)) + d_2 \kappa w}{2 \cos(\omega u) \kappa^2}.$$

By using formulas (7.6) and (7.4) we obtain (4.4).

8. ACKNOWLEDGMENTS

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